

Supplemental Material: Local Superfluid Density

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In Supplemental Material, we define and explain local helicity modulus and local superfluid density. The contents mainly focus on the numerical techniques of quantum Monte Carlo (QMC) simulation. Readers who are interested in only physical results may skip this Supplemental Material.

The helicity modulus Y_{tot} and the superfluid density ρ_s^{HOMO} in a d dimensional *uniform* system [1] are defined by using a winding number vector \mathbf{W} [2] as

$$Y_{\text{tot}} = td\rho_s^{\text{HOMO}} = L^{2-d} \frac{\langle \mathbf{W}^2 \rangle}{\beta}, \quad (1)$$

where t is the "averaged" short-range hopping amplitude, L is a linear size of the system. The α -component W_α of \mathbf{W} stands for the number of winding particles along the α axis in the path-integral formalism, and can be evaluated by QMC method. The value Y_{tot} is usually insensitive to details of the system, but ρ_s^{HOMO} may depend strongly on them such as values of hopping amplitudes and interactions. In fact, for instance, it is well known that the helicity modulus exhibits a universal jump at a Kosterlitz-Thouless (KT) transition point in two dimensions.

Now, keeping in mind the above facts of the uniform systems, let us discuss local superfluidity and local helicity modulus in spatially inhomogeneous systems. To see the universal nature of the systems, we will mainly use the local helicity modulus rather than local superfluid density. In order to theoretically define helicity modulus, we have to impose a periodic boundary condition along at least one spatial direction, because the modulus is defined by the energy variation after slightly twisting the boundary condition. Namely, by definition, it is impossible to define "truly" local helicity modulus at any position \mathbf{x} on the d dimensional space. However, when $d \geq 2$, we can introduce a local helicity modulus defined at any position on one special x direction by imposing a periodic boundary condition along a direction perpendicular to the x axis. For a d -dimensional system with $d \geq 2$, let us define the local helicity modulus $Y(x)$ on x axis such that the total helicity modulus is given by summation of $Y(x)$ along the x direction:

$$Y_{\text{tot}} = \sum_x Y(x). \quad (2)$$

Following Eqs. (1) and (2), we then define the relation between the local superfluid density $\rho_s(x)$ and $Y(x)$ as

$$\rho_s(x) = \frac{Y(x)}{td}. \quad (3)$$

In this equation, $\rho_s(x)$ stands for the superfluid density along a direction perpendicular to the x axis. For example, if we consider a two dimensional system with open boundary condition along the x axis, $\rho_s(x)$ is the superfluid density along the y direction at x .

Next we explain how the local helicity modulus is related to numerical evaluated quantities such as \mathbf{W} . Similarly to local helicity modulus, winding (topological) numbers including \mathbf{W} also has a non-local nature and a periodic boundary condition is necessary along at least one direction to define them. Paying attention to these properties, we can introduce the partial winding number vector $\mathbf{w}(x)$ at each position on the x axis. The summation of $\mathbf{w}(x)$ over the x axis is equivalent to the original winding-number vector \mathbf{W} :

$$\mathbf{W} = \sum_x \mathbf{w}(x). \quad (4)$$

The x component $w_x(x)$ of $\mathbf{w}(x)$, which can be evaluated by QMC, does not satisfy the property of winding number, since information about the whole range of the x axis is necessary to define winding number along the x axis. However, sum of them, i.e., W_x can be a winding number if we impose a periodic boundary condition along the x direction. Each remaining component $w_\alpha(x)$ ($\alpha \neq x$) is the number of winding particles along the α direction at x , and thus it has a topological nature.

From Eqs. (1), (2) and (4), we find that $\mathbf{w}(x)$ and $\rho_s(x)$ should satisfy the following relation,

$$Y(x) = L^{2-d} \frac{\langle \mathbf{W} \cdot \mathbf{w}(x) \rangle}{\beta}. \quad (5)$$

When an open boundary condition is applied along the x axis as in our setup in the main text, the x component of the winding vector becomes zero and $\rho_s(x)$ represents the superfluid density along the y axis at the position x . In this way, we can evaluate the local helicity modulus and local superfluid density (see Fig.2 of the main text).

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Unavoidable Gapless Boundary State and Boundary Superfluidity of Trapped Bose Mott States in Two-Dimensional Optical Lattices

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We study the boundary nature of trapped bosonic Mott insulators in optical square lattices, by performing quantum Monte Carlo simulation. We show that a finite superfluid density generally emerges in the incommensurate-filling (IC) boundary region around the bulk Mott state, irrespectively of the width of the IC region. Both off-diagonal and density correlation functions in the IC boundary region exhibit a nearly power-law decay. The power-law behavior and superfluidity are well developed below a characteristic temperature. These results indicate that a gapless boundary mode always emerges in any atomic Mott insulators on optical lattices. This further implies that if we consider a topological insulating state in Bose or Fermi atomic systems, its boundary possesses at least two gapless modes (or coupled modes) of an above IC edge state and the intrinsic topologically-protected edge state.

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Introduction.— Topological insulators (TIs) [1, 2], more widely, symmetry-protected-topological (SPT) states [3–5], have been vividly studied as new quantum many-body states in the last decade. These gapful states cannot be characterized by any *local* order parameter, while they generally possess a gapless edge/surface mode. Each SPT phase is protected by certain symmetries, namely, it is stable against any perturbation keeping the symmetries. A complete classification of TIs and the relationship between their bulk symmetry and the corresponding surface/edge state have been established for free fermion models [6–8]. Several TI materials have been synthesized and their surface/edge states have been observed [1, 2].

Many physicists stimulated by the study of fermionic TIs have been exploring SPT states in spin and boson systems. The Haldane-gap state [9, 10] of one-dimensional (1D) spin-1 antiferromagnets is a typical SPT state in quantum spin systems, and it is indeed realized in several quasi-1D magnets [11, 12]. In addition to the Haldane state, several SPT phases in 1D fermion, boson and spin systems have been discussed. In fact, a way to classify 1D bosonic SPT phases has been proposed by tensor product representation [13].

On the other hand, two- or three-dimensional (2D or 3D) bosonic SPT phases and their edge/surface states have been little understood. Several theorists discussed the possibility of higher-dimensional bosonic TIs [5, 14–18], and proposed ways to classify them: bosonic TIs in spatial dimensions d can be distinguished by a technique based on $(d + 1)$ th group cohomology [15–18]. In those studies, some models for bosonic TIs were predicted, but it is difficult to realize them in real materials because the corresponding Hamiltonians contain various tuned cou-

pling constants.

For the realization of 2D or 3D SPT phases in boson or spin systems, strong interactions among bosonic particles or spins are generally necessary. The interaction usually makes it quite difficult to analyze the systems, and this is a main reason why the theory for 2D or 3D bosonic TIs has not been developed in comparison with fermionic TIs. Because of the same reason, even *non-topological* (i.e., trivial) gapped phases and their boundary nature have not been understood well in the strongly interacting boson and spin systems. In a sense, boundary nature of gapped states is more important than classification of ground states because physical phenomena at boundary can be observed and their information often provides a experimental way to characterize the bulk state.

Recently, we have studied a edge state of 2D spin-Peierls states [19], by quantum Monte Carlo (QMC) calculations [20–22]. The Peierls state is a typical trivial gapped state in quantum spin systems and it does not accompany any spontaneous breaking of basic symmetries (such as spin rotation and time-reversal symmetries). We showed that if we prepare a sufficiently clean edge of the Peierls state with a large enough length (~ 50 sites), we can observe a gapless Tomonaga-Luttinger-liquid (TLL) like behavior [23] along the edge and the edge spin-spin correlation function decays in an almost algebraic fashion. We proposed some experimental ways of detecting these gapless edge excitations. In this paper, we will explore the fundamental nature of boundary states of 2D Bose Mott insulator on optical lattices, by QMC computations. Similarly to the spin-Peierls state and fermionic TIs, no spontaneous symmetry breaking occurs and a finite bulk excitation gap exists in Bose Mott states. They

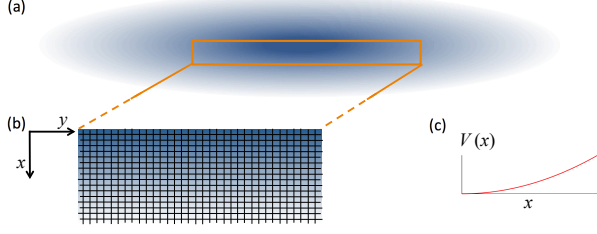


FIG. 1: (color online) (a) Full region of a 2D trapped Bose system on a square lattice. (b) Quasi-1D geometry we consider and (c) the corresponding confinement potential. Density of color stands for the depth of chemical potential.

have been already realized in ultracold-atomic systems on optical lattice [24–28]. Therefore, their boundary nature could be an important research subject as a good comparison in that of bosonic TIs.

An important feature of trapped ultracold-atom systems is that their boundary is always clean. This considerably contrasts with solid systems, whose boundary is usually dirty. As a result, we always observe a clean and homogeneous boundary region in Bose Mott states. We will numerically clarify the boundary properties of 2D Bose Mott states. They could be experimentally detected in principle. Our findings are also useful to deeply understand boundary states of cold-atom TIs as well as those of Bose Mott states.

Model.— In this paper, we focus on the 2D soft-core Bose Hubbard model with confinement potentials. To discuss the finite-size effects systematically, we consider systems on the quasi-1D geometry shown in Fig. 1(b). This geometry would be hard to be realized in optical lattices, but it could be regarded as a boundary part of circular or elliptic shaped trapped systems [see Fig. 1(a)]. The Hamiltonian for the quasi-1D geometry is given as

$$\mathcal{H} = -t \sum_{x,y} (b_{x,y} b_{x+1,y}^\dagger + b_{x,y} b_{x,y+1}^\dagger + h.c.) + U \sum_{x,y} n_{x,y}^2 - \sum_{x,y} V(x) n_{x,y}, \quad (1)$$

where $V(x) = \mu_0 + \alpha x^2$, $n_{x,y} = b_{x,y}^\dagger b_{x,y}$ and $b_{x,y}$ ($b_{x,y}^\dagger$) is a boson creation (annihilation) operator at position (x, y) . Parameters t , U , and $V(x)$ denote hopping amplitude, on-site repulsion, and axial confinement potential along the x -axis direction, respectively. To realize the quasi-1D geometry, we impose the periodic (open) boundary condition along the y (x) direction. In our computations, we fix $U/t = 20$, at which the bulk system can belong to the Mott-insulating state with a single boson per site [24–28]. We also fix the x -direction length $L_x = 48$, but tune the y -direction length L_y . Increase of α means the growth of potential slope between bulk Mott and vacuum (empty) regions.

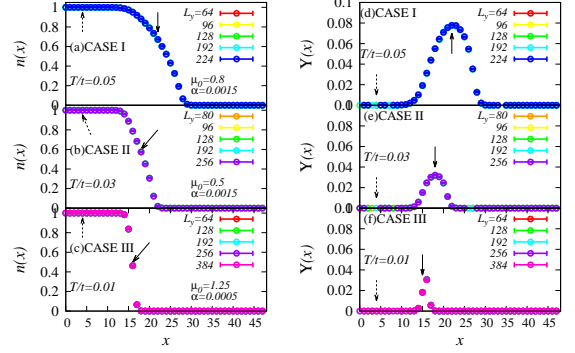


FIG. 2: (color online) (a)-(c) Density and (d)-(f) stiffness (\propto superfluid density) profiles estimated by QMC calculations at extremely low temperatures T . Pairs [(a),(d)], [(b),(e)] and [(c),(f)] are the results of CASEs I, II and III of Table I, respectively. Solid (dotted) arrows denote positions of x_0 (x_1) in Table I. Results of systems with different sizes L_y are almost degenerate.

	μ_0/t	α/t	x_0/L_x	x_1/L_x	Δx
CASE I	0.8	0.0015	0.458	0.0833	21 sites
CASE II	0.5	0.0015	0.375	0.0833	10 sites
CASE III	1.25	0.005	0.333	0.0833	4 sites

TABLE I: Three parameter setups we chose, CASEs I, II, and III. The last three columns x_0/L_x , x_1/L_x and Δx denote representative positions in the incommensurate filling (IC) and the Mott regions, and the width of the IC region, respectively (see the text and Fig. 2).

Boundary state in $T \rightarrow 0$ limit.— In order to understand the boundary nature of the Bose Mott state, we will study particle densities, superfluidity, and correlation functions of the model (1) by QMC computations. In Fig. 2, we first show the local density profile $n(x) = \langle n_{x,y} \rangle$ and local helicity modulus $Y(x)$, which is proportional to the local superfluid density [29, 30], changing μ_0 and the curvature α at very low temperatures T (k_B is set to be unity). We here show QMC results of three parameter settings (μ_0, α) in Table I as representatives. In all CASEs I, II and III, an incommensurate (IC) filling region (e.g., $0.21 < x/L_x < 0.6$ in CASE I) appears between the filling-one Mott and the vacuum (empty) states. In the IC region, the local superfluid density takes a finite value. Size of the IC region and the superfluid density profile are almost irrespectively of the length L_y when L_y is sufficiently large. We note that finite-size effect along x direction can be ignored in the present parameter settings. Survival of a superfluid density sharply contrasts with the case

of the purely 1D Bose system because the latter superfluid density is known to disappear in the thermodynamic limit [33–35]. We confirmed that a further narrower IC region still survives when a more large value of α is applied. Furthermore, we observe an IC region when we apply other types of the chemical potentials with non-harmonic curvatures [36, 37]: $V(x) = \mu_1 + \alpha_1 x^{10}$ and $= \mu_2 + \alpha_2 \exp(-x/\xi_2)$. These results indicate that an IC superfluid region between Mott and vacuum areas generally appears and a special potential $V(x)$ with an extremely large curvature is necessary to remove the IC region.

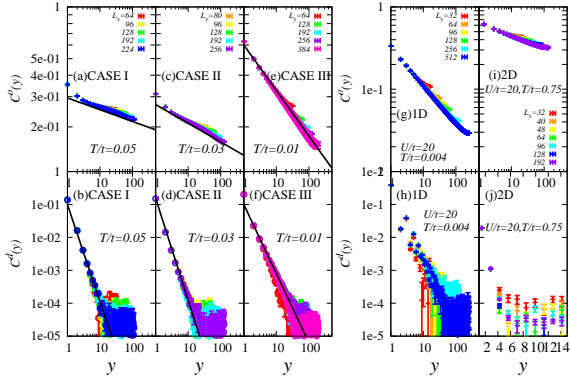


FIG. 3: (Color online) Off-diagonal and density correlation functions along the y direction. Pairs [(a),(b)], [(c),(d)] and [(e),(f)] are the results of CASE I, II, and III at the IC position $x = x_0$, respectively. Pairs [(g),(h)] and [(i),(j)] are respectively the results of spatially uniform 1D and 2D Bose Hubbard models at an IC filling. Black lines are guides to eyes.

In Fig. 3, we present the equal-time one-particle (off-diagonal) correlation function $C^o(y) = \langle b_{x_0,y}^\dagger b_{x_0,0} \rangle$ and density one $C^d(y) = \langle n_{x_0,y} n_{x_0,0} \rangle - \langle n_{x_0,y} \rangle^2$ at the boundary position $x = x_0$ where $\rho_s(x_0)$ takes the largest values. As a comparison, we also show the QMC results of a purely 1D Bose Hubbard model [Fig. 3(g) and (h)] and a spatially uniform 2D Bose Hubbard one [Fig. 3(i) and (j)] in an IC-filling case. The 1D and 2D Bose systems of Fig. 3 belong to TLL and Kosterlitz-Thouless (KT) phases, respectively. At the position x_0 , power-law decays along the y direction are observed in both off-diagonal and density correlations with long distances. Their critical exponents are evaluated by assuming the form $C^z(y) = \text{const.} \times y^{-\eta_z}$, and they are summarized in Table II. The emergence of algebraic decay is independent of the width of IC region. This clearly indicates that at least one gapless edge mode around the bulk Mott-insulating region always appears at very low temperatures. The algebraic decay of the density correlation is quite different from that of the KT phase in uniform

	CASE I	CASE II	CASE III	1D
η_o	0.069(2)	0.12(4)	0.25(1)	0.443(8)
η_d	2.9(1)	3.1(2)	2.1(1)	2.23(6)

TABLE II: Estimated decay exponents for off-diagonal and density correlations, assuming $C^z(y) \sim \text{const.} \times y^{-\eta_z}$, where $z = o$ (d) stands for the off-diagonal (density) correlation.

2D Bose systems. In fact, Fig. 3(j) shows that the density correlation decays exponentially in the 2D case. In addition, it is known [23] that two critical exponents satisfy $\eta_o \eta_d = 1$ in the purely 1D TLL (see Table II), while the relation is clearly broken in the present boundary gapless mode. These results conclude that the boundary IC region possesses intermediate properties between 1D and 2D Bose systems.

Boundary state in finite temperatures.— Next, we discuss the temperature dependence of the boundary IC states. In the present model as well as real experimental systems, effects of finite size and spacial inhomogeneity may spoil true phase-transition phenomena in the thermodynamic limit, but their residual things might still survive. Figure 4 shows the temperature dependence of local helicity modulus $Y(x_0)$ at a typical IC position $x = x_0$ in CASE I. The figure shows that the L_y dependence of $Y(x_0)$ becomes negligibly small below $T/t \sim 0.075$, where off-diagonal and density correlation functions decay algebraically. This small L_y dependence implies the existence of a gapless KT-like phase around the bulk Mott state.

To quantitatively determine a KT-transition-like temperature in our finite inhomogeneous system, we simply apply the standard finite-size analysis for the KT transition in spatially uniform 2D systems, which is expected to be reliable if the width of the IC region is sufficiently large as in CASE I. In the uniform system, Y approaches to $2k_B T_{KT}/\pi$ at the KT transition temperature $T = T_{KT}$. For each finite system with size L , the KT transition

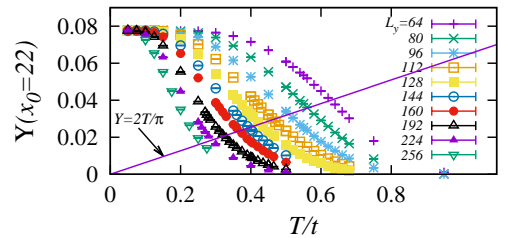


FIG. 4: (color online) Local helicity modulus at a IC position $x = x_0$ in CASE I.

temperature $T^*(L)$ is known to be

$$T^*(L) = T_{KT}(L \rightarrow \infty) \left(1 + \frac{1}{2 \ln L + C} \right), \quad (2)$$

where C is a fitting parameter. Since we have the data of $Y(L_y)$ for different sizes L_y in Fig. 4, the tempera-

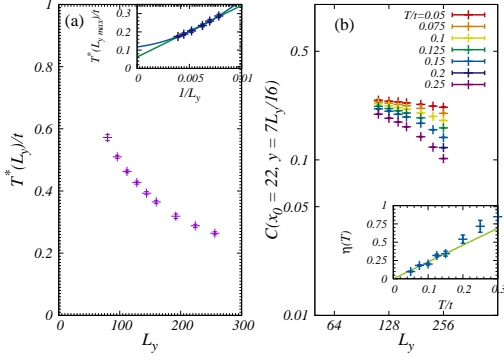


FIG. 5: (a) Size dependence of characteristic temperature $T^*(L_y)$. (b) Temperature dependence of the exponent η_o .

ture $T^*(L_y)$ can be estimated as the cross point between numerically determined $Y(L_y)$ in Fig. 4 and the linear line $Y(T) = 2k_B T/\pi$. In Fig. 5(a), we plot the evaluated $T^*(L_y)$. In its inset, we determine the value of $T^*(L_y \rightarrow \infty)$ by combining $T^*(L_y)$ and the scaling relation (2) ($T^*(L_y \rightarrow \infty)$ corresponds to the KT transition temperature T_{KT} in the case of uniform systems). The characteristic temperature $T^*(\infty)$ is determined as $T^*(\infty)/t \sim 0.11(1)$.

As an alternating way to determine $T^*(\infty)$, we can utilize correlation functions in our inhomogeneous system. It is well known that the critical exponent η_o of the off-diagonal correlator increases from zero and it becomes a quarter at the KT transition with the growth of temperature. Let us simply apply this property to fix the KT-like temperature in our IC region. The inset of Fig. 5(b) is the T dependence of the exponent η_o . We see that η_o indeed crosses a quarter around $T = T^*(\infty)$ which was estimated above from $Y(L_y)$.

We stress that the temperature $T^*(\infty)$ is much lower than the true KT transition temperature T_{KT} in the uniform 2D system. From the QMC calculation, we obtained $T_{KT}/t \sim 0.92(3)$ for $U/t = 20$ and $\mu/t = -0.74$, where the averaged particle number per site is almost same as that at the position $x = x_0$ in CASE I. This must be because the development of off-diagonal correlation along the x direction is suppressed owing to the existence of Mott-insulating and vacuum regions. When the width of the IC region is small as in CASE III, it is hard to quantitatively determine T^* . However, even in such a case, a KT-like power law in correlations appears at very low temperatures (see Fig. 3).

Structure factors.— From all the discussions above, we see that at least a gapless IC state always appears around the Bose Mott state if temperature is low enough. Finally we discuss a experimental way to detect the gapless edge mode. In cold-atomic systems, the momentum distribution of correlation functions [38] can be observed in principle. For example, time-of-flight (TOF) method and light-scattering spectroscopy have been applied to

observe them. In Fig. 6, we show the momentum- q_y distribution of $S^o(x, q_y) = 1/\sqrt{L_y} \sum_y C^o(x, y) e^{-iyq_y}$ for the IC region at $x = x_0$ and for the bulk Mott region at $x = x_1$. Here, $C^o(x, y) = \langle b_{x,y}^\dagger b_{x,0} \rangle$. In the realistic experimental setup, the number of sites along the y -axis is less than ~ 100 sites and then we set $L_y = 64$ in all the panels of Fig. 6. As temperature decreases, the mo-

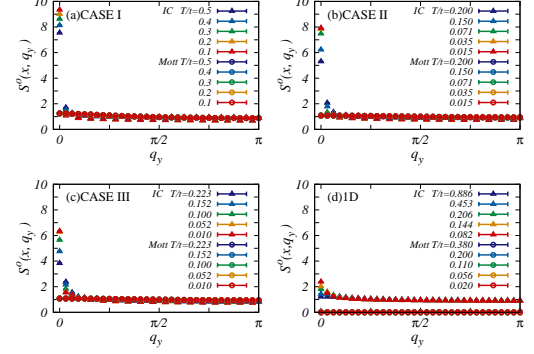


FIG. 6: (color online) (a)-(c) T dependence of structure factors $S^o(x, q_y)$ at $L_y=64$. Circles (triangles) are the results for the IC (Mott) region at $x = x_0$ ($x = x_1$). (d) T dependence of the structure factor of the off-diagonal correlator $S^o(q)$ in a TLL state of 1D Bose Hubbard model.

mentum distribution at zero wave number $q_y = 0$ of the IC region well develops, while that of the Mott region is suppressed for any wave number q_y . The $q_y = 0$ peak reflects the development of superfluidity in the IC region. In Fig. 6 (d), as a comparison to the IC region, we show the momentum distribution of a finite-size 1D Bose Hubbard model under an uniform chemical potential with the almost same filling as the IC boundary region. In the 1D case, we also observe a $p_y = 0$ peak structure which is the contribution of TLL. From Fig. 6, we find that momentum distributions in both Mott and IC regions exhibit the similar T dependence to the finite-size 1D system with the same filling. This is an another evidence for the existence of a gapless edge mode in the IC region and it also indicates the difficulty of distinguishing the IC gapless state and the 1D TLL.

Summary and discussions.— In conclusion, we have studied the edge state surrounding the 2D Bose Mott-insulating phase. From the QMC method, we have found that in the IC edge region, both off-diagonal and density correlators show an algebraic decay and a superfluid density appears below a characteristic temperature irrespective of the width of the IC region. This "universal" gapless edge mode can be detected e.g., by observing a $q_y = 0$ peak of $S^o(x, q_y)$.

Our result naturally indicates that a similar gapless edge mode generally emerges in any kinds of 2D cold-atomic Bose and Fermi insulating states. Therefore, if we consider a topological insulating state in 2D cold-

atom systems, we can expect that there are at least two gapless modes of the edge state in the IC region and an intrinsic topologically-protected edge state as shown in Fig. 7. There might be a relevant coupling between these two edge states. Thus, when we discuss a way to detect topological edge mode in 2D cold-atom systems, we should generally consider effects of a non-topological (but universal) edge mode in the IC region around the bulk insulating area.

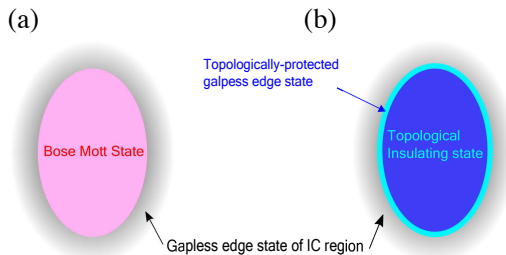


FIG. 7: (color online) Spatial structures of a trapped Bose Mott state (a) and a trapped topological insulating state (b) in 2D cold atoms.

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